Combustion overview and requirements

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APDEC-II ISIC Kick-off Meeting
Perseverance Hall, LBNL
October 18-19, 2006

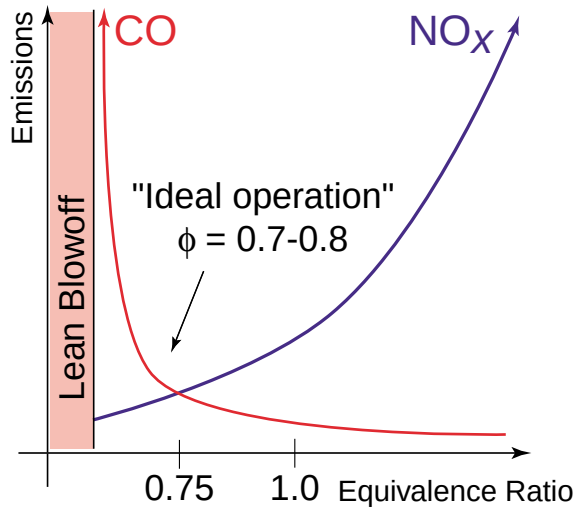
Outline of Talk

1. Overview of problem setting
2. Solution approach, algorithm components
3. Two examples from current research
4. Future research directions, requirements

Lean Premixed Turbulent Combustion

Reduced emissions in domestic and industrial furnaces and burners

1. Lean: Low emissions
2. Turbulence: wrinkled flame surface $\longrightarrow$ compact devices

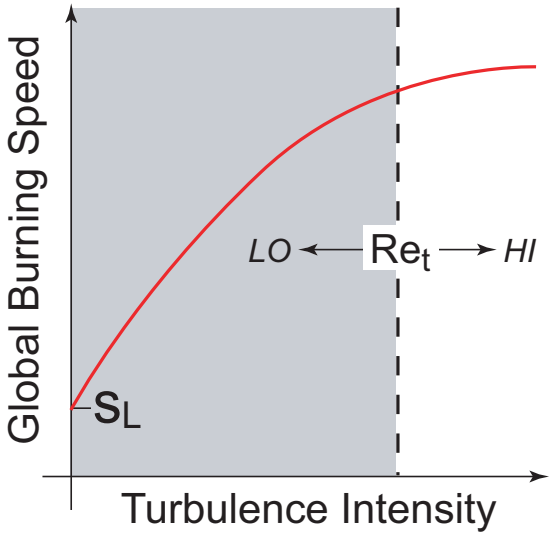


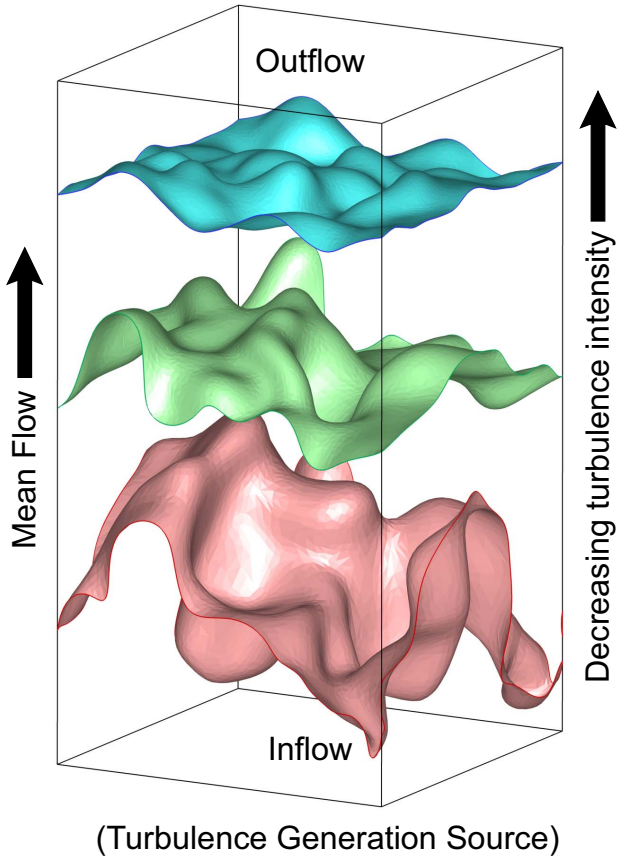
But...

- Flame density practically limited by intra-flame interactions, dilatation, Kolmogorov scales
- Stabilization difficulties (see next slide)
- Safety issues (flashback)

Flame Propagation in Spatially Decaying Turbulence

Global consumption rate increases with turbulence-generated flame area





If mean inflow not precisely matched to global burning speed, not stationary

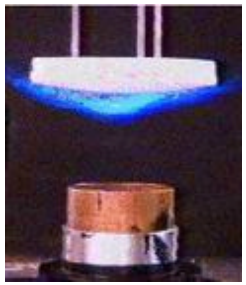
- Flame moves away: less wrinkles, reinforces downstream drift, blowoff
- Flame moves closer: more wrinkles, reinforces upstream drift, flashback

Natural flame instability makes this configuration non-stationary.

Taxonomy of Related Experiments


Oblique Flames

Jet engine after-burners, commercial furnaces



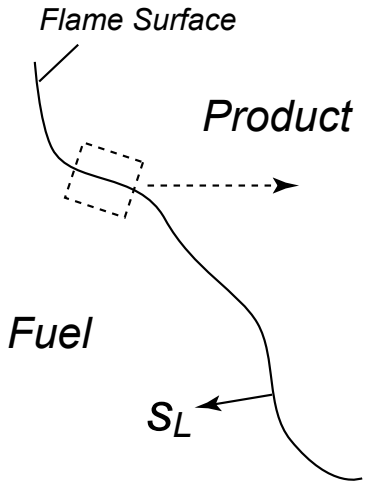

Unattached Flames

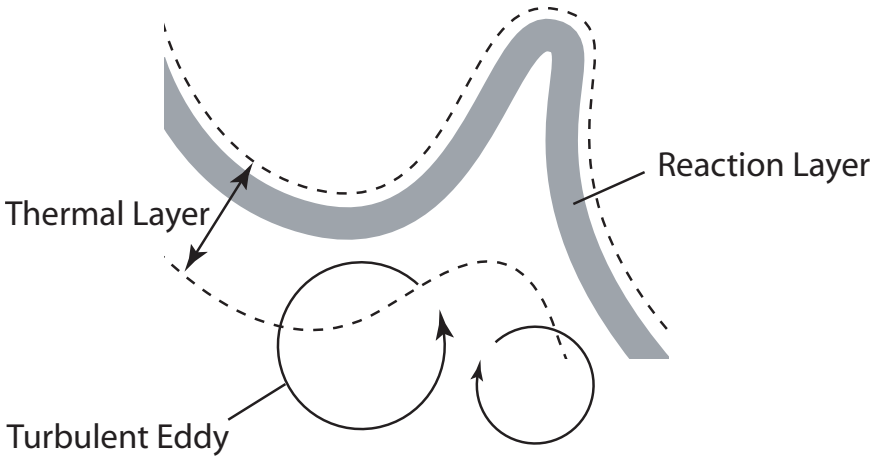
Diamond deposition, industrial boilers


Envelope Flames

Domestic/commercial air furnaces

Flame and Turbulence Scales: Definitions



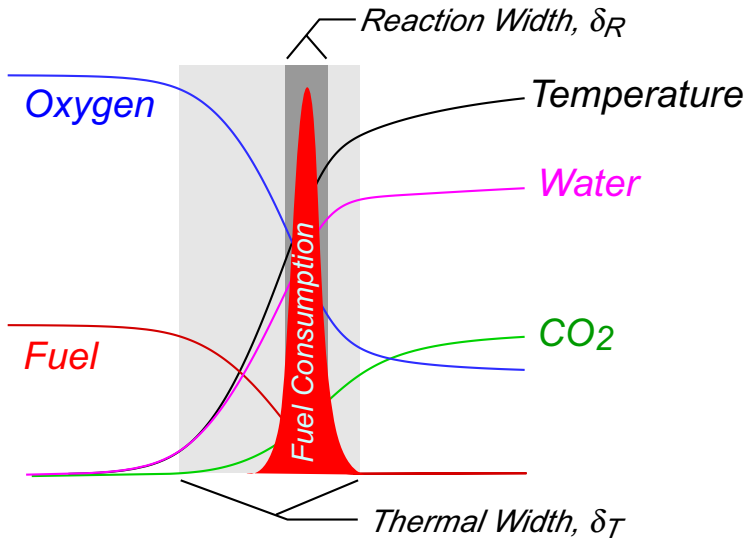


Flame scales:

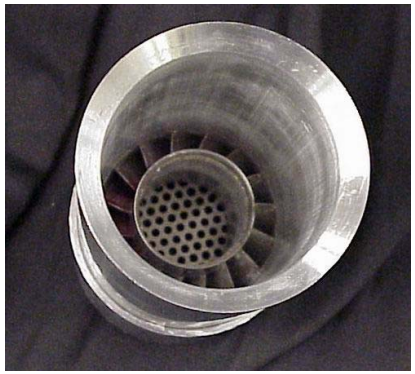
- Flame (thermal) width, δ_T
- Laminar burning speed, s_L

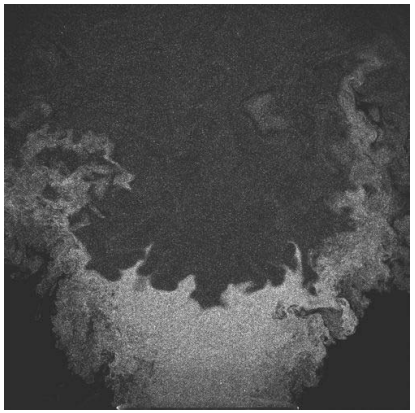
Turbulence scales:

- Energy-bearing eddy size, ℓ_t
- RMS fluctuation intensity, u'



Relevant Scales





- Geometry (cm): $\sim 5 - 10$
- Flow/Acoustic Speed (m/s): $\sim 3/350$
- Turbulence intensity (% flow speed): 5
- Flame (μm): $\delta_T/\delta_R \sim 800/150$
- Turbulence (μm): $\eta/\ell_t \sim 220/3000$

Objective

Simulate laboratory-scale turbulent premixed combustion using detailed kinetics and transport without subgrid models for turbulence or turbulence-chemistry interaction

Purpose:

- Basic turbulent flame dynamics
- Model development and calibration

Traditional approach: Compressible DNS

- High-order explicit finite-difference methods
- At least $O(10^{12})$ zones
- At least $O(10^{6})$ timesteps
- 10-100 chemical species, tens$\sim$hundreds reactions

Limited to sugar-cube-sized domains

Approach

Observation:

- Open laboratory turbulent flames are low Mach number
- Regions requiring high-resolution are localized in space

Our approach:

- Low Mach number formulation
  - Eliminate acoustic time-step restriction while retaining compressibility effects due to heat release
  - Conserve species and enthalpy
- Adaptive mesh refinement
  - Localize mesh where needed
  - Complexity from synchronization of elliptic solves
- Parallel architectures
  - Distributed memory implementation
  - Dynamic load balancing of heterogeneous work load

Low Mach Number Combustion

Low Mach number model, $M = U/c \ll 1$ (Rehm & Baum 1978, Majda & Sethian 1985)

Start with the compressible Navier-Stokes equations for multicomponent reacting flow, and expand in the Mach number, $M = U/c$.

Asymptotic analysis (matching terms in powers of M):

$$p(\vec{x}, t) = p_o(t) + \pi(\vec{x}, t) \quad \text{where} \quad \pi/p_o \sim \mathcal{O}(M^2)$$

- p_o does not affect local dynamics, π does not affect thermodynamics
- For open containers p_o is constant
- Acoustic waves analytically removed

Constrained combustion system evolution

Low Mach number flows evolve with $Dp_o/Dt \sim 0$.

$$\begin{aligned}
\rho\frac{\partial U}{\partial t} + \rho(U\cdot\nabla)U + \nabla\pi &= \mathcal{D}_U \\
\frac{\partial(\rho Y_m)}{\partial t} + \nabla\cdot(\rho U Y_m) &= \mathcal{D}_m + \mathcal{R}_m \\
\frac{\partial(\rho h)}{\partial t} + \nabla\cdot(\rho U h) &= \mathcal{D}_h
\end{aligned}$$

The equation of state, $p_o = \mathcal{F}(\rho, T, Y_m)$, allows us to use continuity

$$\nabla\cdot U = S = \frac{1}{\rho}\frac{D\rho}{Dt}$$

to express the pressure condition in terms of a constraint on the velocity field divergence, S. Incorporating the constraint into the U evolution, mass and energy may be integrated with robust conservative discretizations.

Projection Method for Constrained Evolution

Note: Any vector field V can be written as

$$V = U_d + \nabla\phi$$

where $\nabla \cdot U_d = 0$. Define projection, $\mathbf{P}$, such that $U_d = \mathbf{P}V$

Projection algorithm example:

$$U_t + U \cdot \nabla U + \nabla\pi = 0, \qquad \nabla \cdot U = 0$$

1. Advection step, $U^* = U^n - \Delta t\ U\nabla \cdot U$
2. Projection step, $U^{n+1} = \mathbf{P}U^*$

Procedure recasts system to an initial value problem

$$U_t + \mathbf{P}(U \cdot \nabla U) = 0$$

2nd Order Fractional Step Scheme

1. Conservatively advance species mass and energy

$$\frac{\rho^{n+1}\chi^{n+1} - \rho^n\chi^n}{\Delta t} + \nabla\cdot(\rho U^{ADV}\chi)^{n+\frac{1}{2}} = \mathcal{D}_\chi + \mathcal{R}_\chi \quad \text{for } \chi = h, m$$

   Use Strang approach to split chemistry and diffusion integration (e.g. use VODE and Crank-Nicolson, resp.) Here, $\rho = \sum \rho Y_m$ and $h = \sum h_m(T) Y_m$.

2. Construct an intermediate velocity field U^* using a lagged pressure gradient:

$$\rho^{n+\frac{1}{2}} \frac{U^* - U^n}{\Delta t} = -\left(\rho[U^{ADV}\cdot\nabla U]\right)^{n+\frac{1}{2}} - \nabla\pi^{n-\frac{1}{2}} + \mathcal{D}_U$$

3. Compute $S(\rho,\chi)^{n+1}$, and decompose U^* to extract the component satisfying the divergence constraint.

Enforce the constraint

Velocity decomposition is achieved by solving

$$\nabla \cdot \left(\frac{1}{\rho} \nabla \phi \right) = \nabla \cdot U^* - S^{n+1}$$

for ϕ, and setting

$$\pi^{n+1/2} = \pi^{n-1/2} + \phi$$

and

$$U^{n+1} = U^* - \frac{1}{\rho} \nabla \phi$$

This is a variable-coefficient linear solve

Conservative Integration

Godunov-based finite-volume discretization requires velocity at cell faces

- Start with $U^n = (u, v)^n, \rho^n, Y_m^n, h^n$ at cell centers
- Predict normal velocities and all states at cell faces
- MAC-project the edge-based normal velocities, i.e. solve

$$D^{MAC}(\frac{1}{\rho^n} G^{MAC} \psi) = D^{MAC} U^{n+1/2} - S^{n+1/2}$$

and define normal advection velocities

$$\begin{aligned} u^{ADV}_{i+1/2,j} &= u^{n+1/2}_{i+1/2,j} - \frac{1}{\rho^n} G^x \psi, \\ v^{ADV}_{i,j+1/2} &= v^{n+1/2}_{i,j+1/2} - \frac{1}{\rho^n} G^y \psi \end{aligned}$$

Advection velocities must satisfy the constraint

Algorithm Overview

Algorithm Components

Data: Cell-centered, uniform grid
Advection: Explicit Godunov with projected velocities
Diffusion: Crank-Nicolson
Projection: ρ-weighted projection for elliptic constraint
Chemistry: Stiff ODE integrator (VODE)

Global linear algebra:

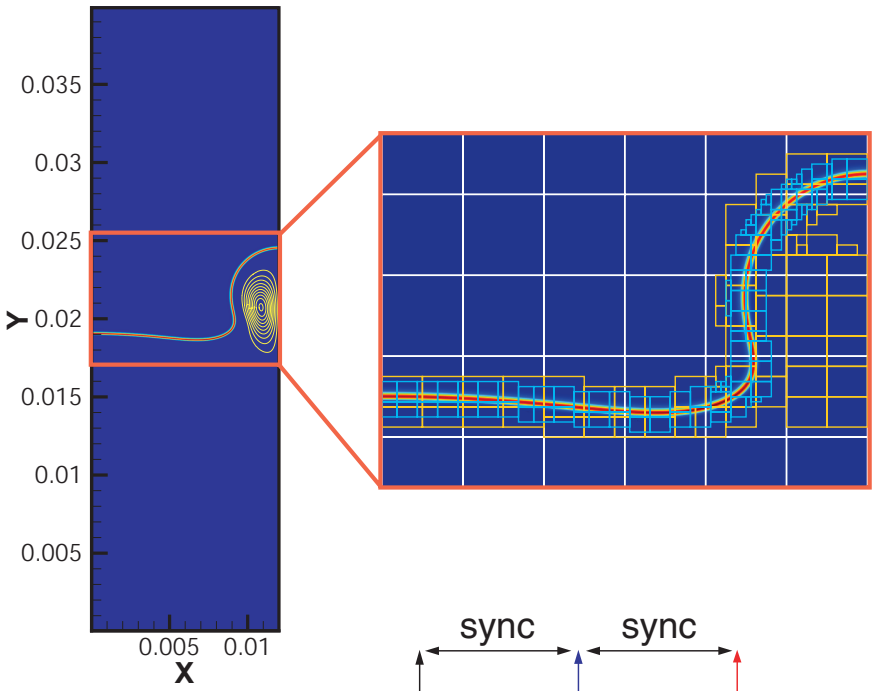
1. MAC velocities (scalar, cc)
2. Species diffusion (scalar (coupled), cc)
3. Heat conduction (scalar (coupled), cc)
4. Momentum viscosity (coupled, cc)
5. Velocity projection (scalar, nc)

AMR - Grid Structure and Time Advance

Block-structured hierarchical grids

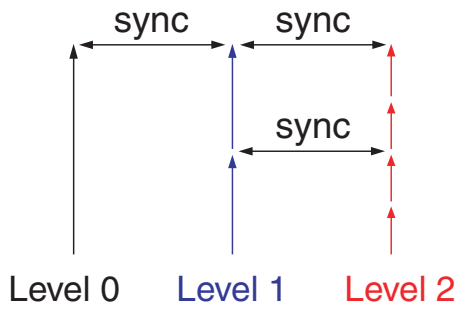
Each grid patch (2D or 3D)

- Logically structured, rectangular
- Refined in space and time by evenly dividing coarse grid cells
- Dynamically created/destroyed to track time-dependent features



Subcycled time integration:

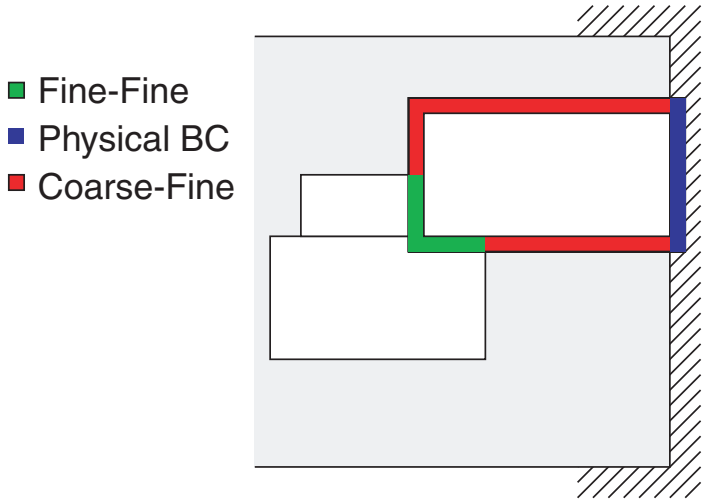
- Advance level ℓ, then
  - Advance level $\ell + 1$
    level ℓ supplies boundary data
  - Synchronize levels ℓ and $\ell + 1$



AMR Synchronization

Coarse grid supplies Dirichlet data as boundary conditions for the fine grids.

Errors take the form of flux mismatches at the coarse/fine interface, $\delta\Omega_{c-f}$.



Design Principles:

- Define what is meant by the solution on the grid hierarchy.
- Identify the errors that result from solving the equations on each level of the hierarchy “independently” (motivated by subcycling in time).
- Solve correction equation(s) to “fix” the solution.
- For subcycling, average the correction in time.

Synchronizing AMR Levels

Synchronization: Repair flux mismatch along $\delta\Omega_{c-f}$. Correction equations match the structure of the process they are correcting.

- For time-explicit discretizations of hyperbolic components, the correction is explicit and localized at $\delta\Omega_{c-f}$
- For elliptic components (e.g., the projection) the source is localized on $\delta\Omega_{c-f}$ but an elliptic equation is solved to distribute the correction through the domain. Discrete analog of a layer potential problem.
- For discretization of parabolic components, the source is localized on $\delta\Omega_{c-f}$ but the correction equation diffuses the correction throughout the domain over the coarse time step.

Performing corrections for each step of the low Mach number projection algorithm guarantees that the adaptive algorithm preserves the properties of the single grid scheme.

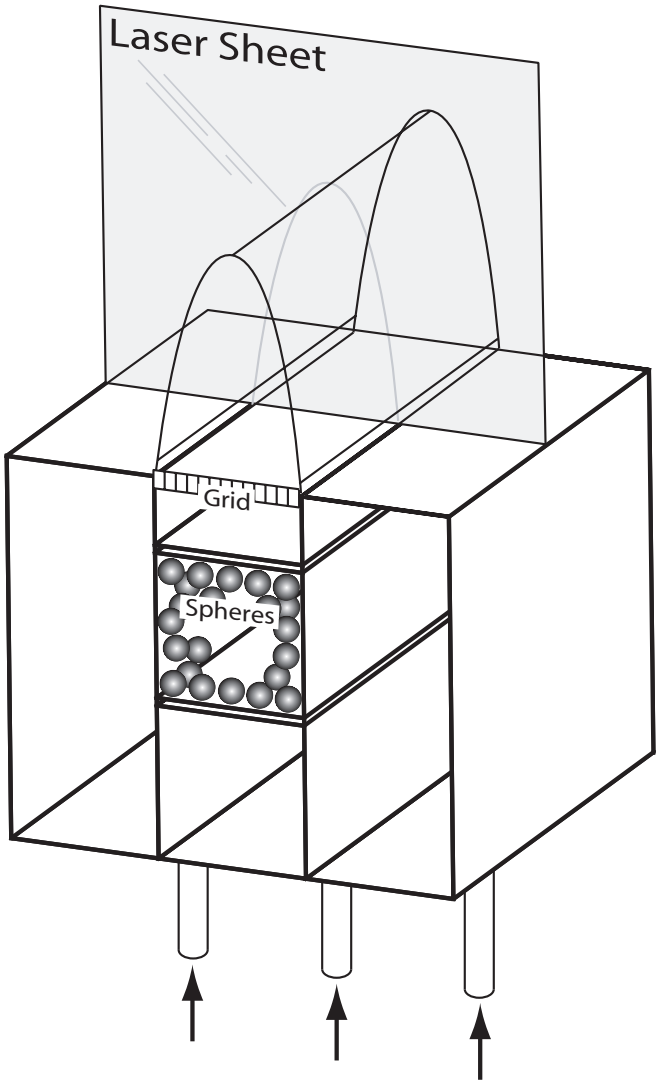
Example Lab-scale applications

Current application studies underway using this parallel adaptive projection methodology:

- Slot Flame (with J. Driscoll, U. Michigan)
  - Stable, continuous envelope flame surface
  - Flame surface statistics to validate experimental data processing
- Swirl Flame (with R. Cheng and I. shepherd, LBNL)
  - Unattached discontinuous flame surface
  - Explore turbulence/chemistry interaction processes where experimental processing techniques fail
  - Current studies performed using idealized configuration (discussed later)

Slot Flame - Objective

Simulate slot burner using detailed kinetics and transport.
Validate 2D planar diagnostics for flame surface statistics.



- Slot dimension: 2.5 $\times$ 5 cm (x3)
- Center slot: Turbulent fuel
  - CH_4/air ($\phi = 1$)
  - Mean inflow: 3 m/s
  - Integral scale: 5.2 mm
  - Intensity: 10%
  - Kolmogorov scale: 200 μm
- Side slots: Laminar pilots
  - Burner stabilized flames
  - Isolate flame from lab
- Diagnostics: PIV and CH-PLIF

Simulation parameters

Nozzle (fuel):

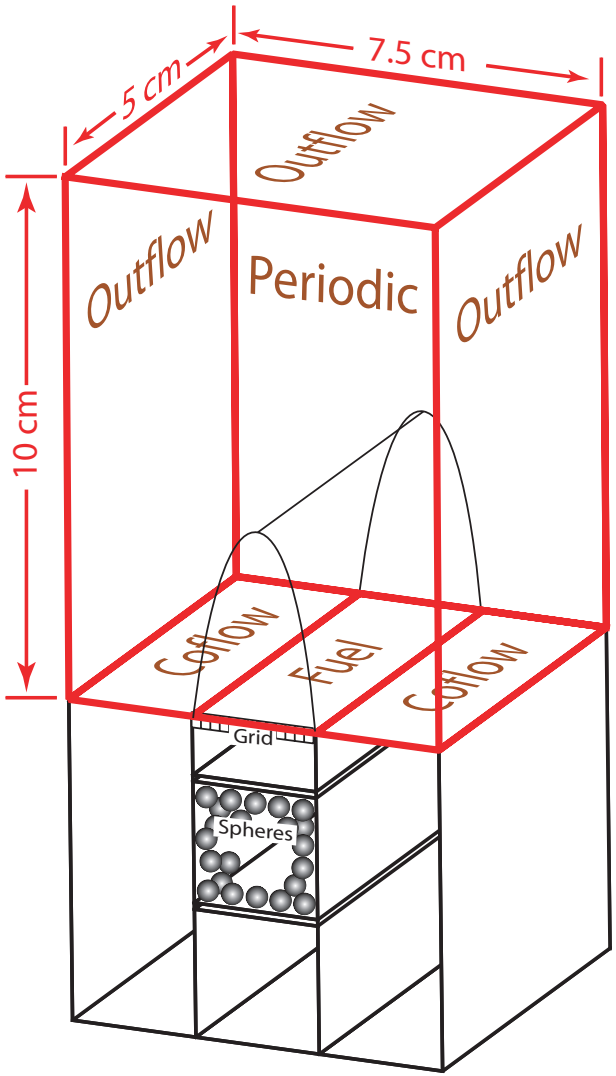
- $\phi = 1$, CH_4-air, $\bar{u} = 3$ m/s*
- Treat as t-dep boundary values
- Evolve fluctuations separately, match experimental (ℓ_t, u')*

Coflow (pilot):

- Hot products at 7 m/s*

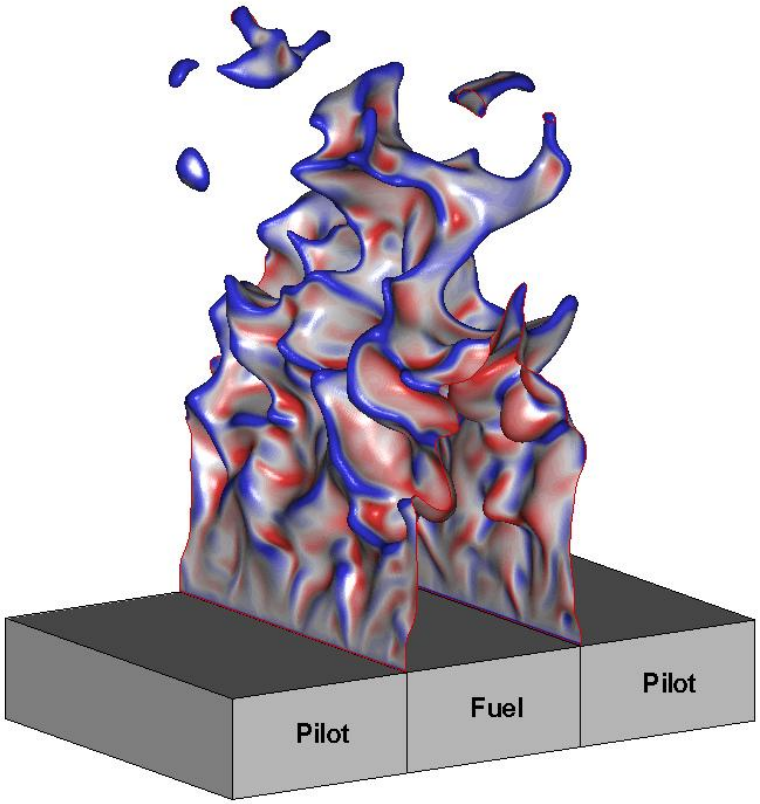
Model:

- DRM-19 (20 species + 84 rxns)
- 3-level dynamic AMR hierarchy
  - 625 μm downstream, coflow
  - 312.5 μm on inlet turbulence
  - 156.25 μm at flame surface

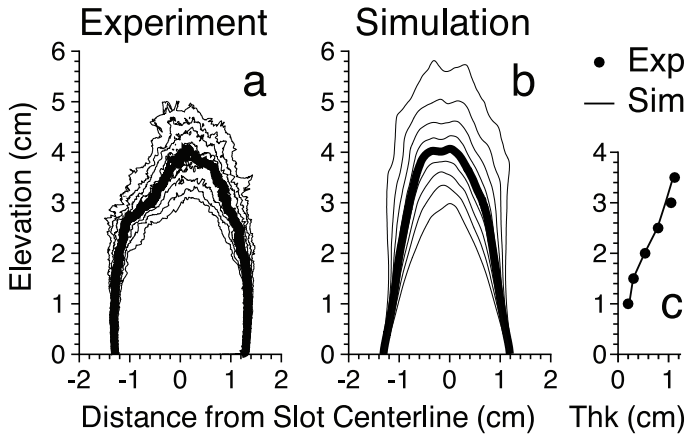


More detail in these characterizations is desireable

Flame surface



Simulated flame surface colored by local mean curvature



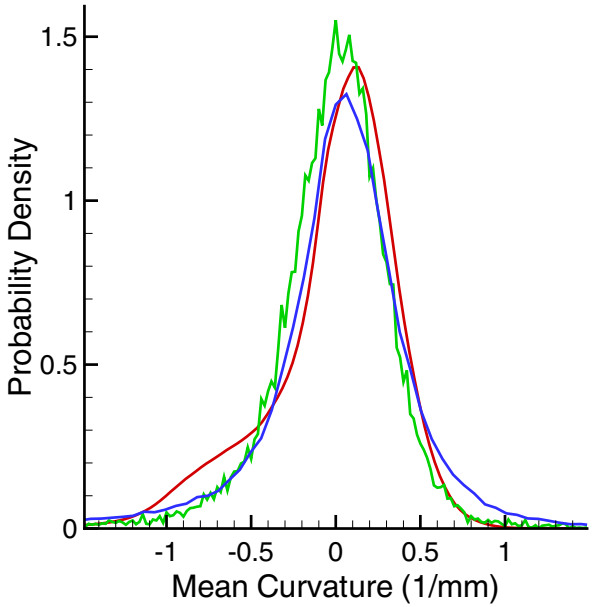
Mean reaction progress, brush thickness

- Turbulent flame speed: expt / sim $\sim$ 1.04
- Brush width agrees for $z < 3.5$ cm

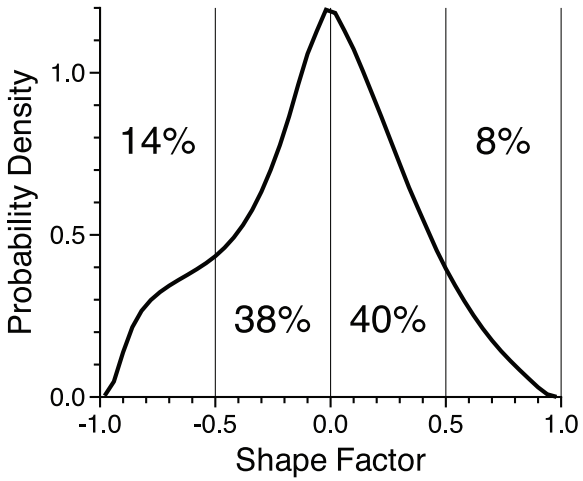
Slot Flame Curvature Statistics

Experimental PIV/PLIF diagnostics are planar.

- How to interpret 2D diagnostics of a 3D field?
- Does the flame behave locally 2D?

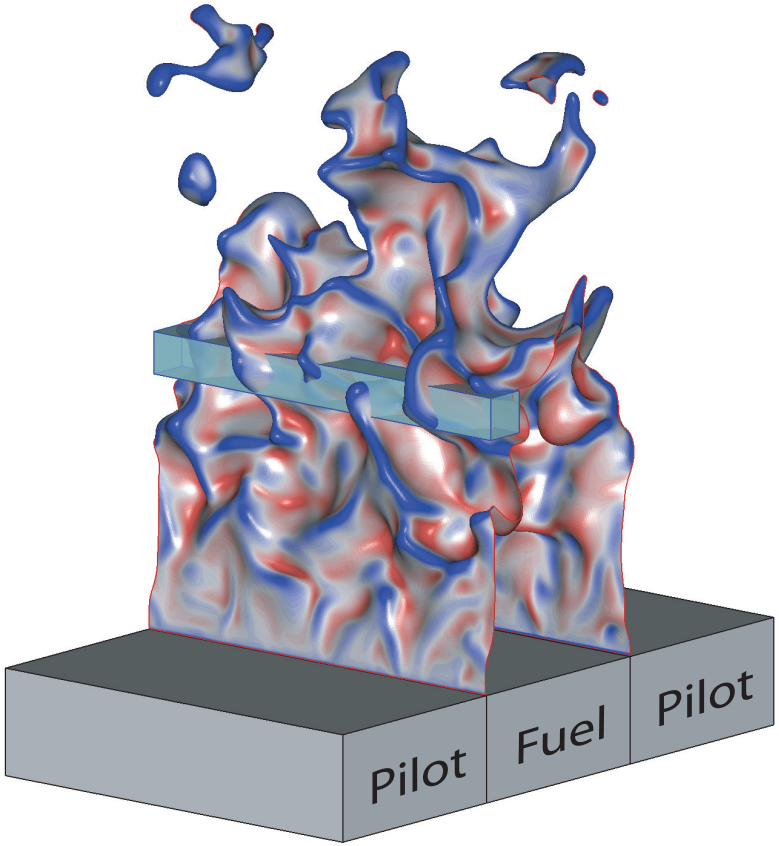


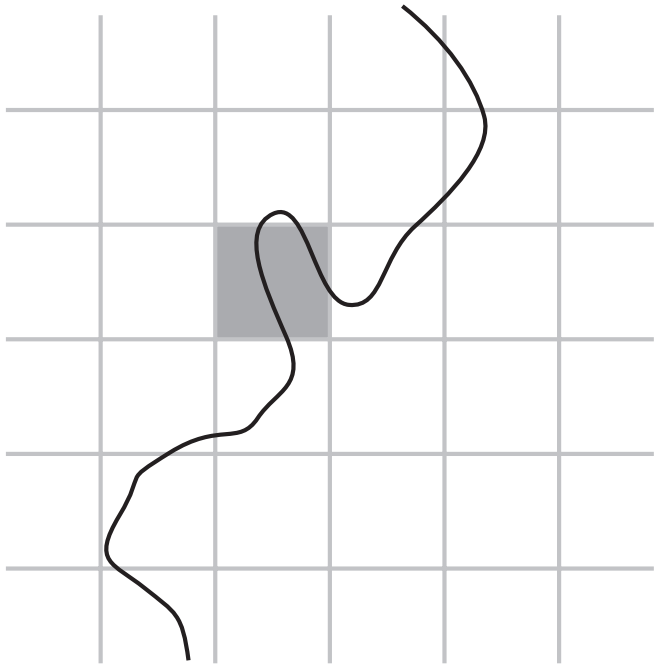
$M = \kappa_{min} + \kappa_{max}$
(B=2D, R=3D, G=Expt)



$S = \kappa_{min}/\kappa_{max}$
("$S = 0 \rightarrow$ locally 2D")

2D and 3D flame surface density

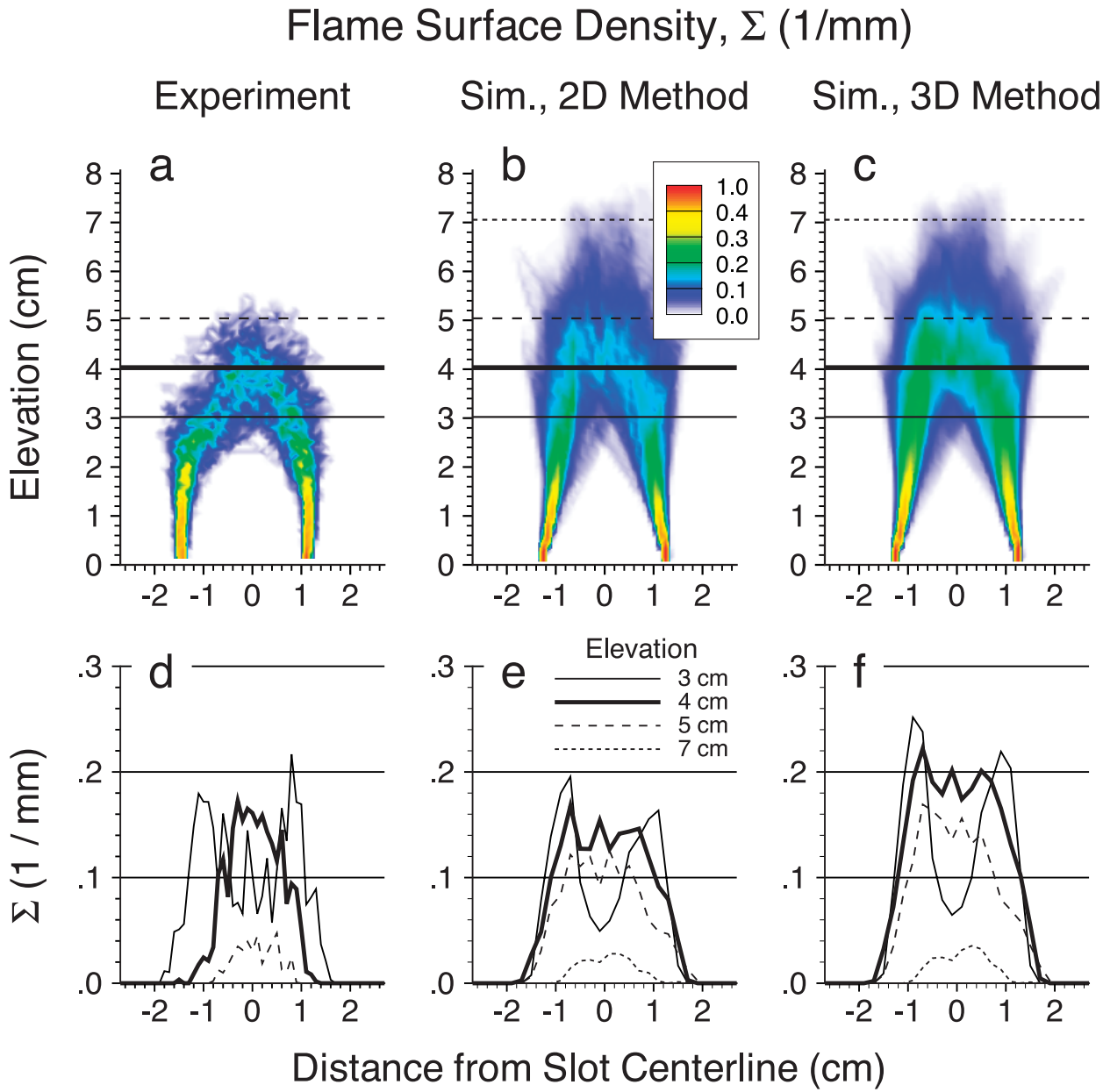




$$\Sigma = \frac{\text{flame area}}{\text{bin volume}}$$

$$\Sigma_{2D} = \frac{\text{flame length}}{\text{bin area}}$$

Flame Surface Density



Descrepancies with comparisons

The computed flame surface statistics are numerically resolved

- Further grid refinements, no changes in statistics
- The flame brush growth, mean flame height, 2D curvature and flame surface statistics show reasonable agreement with experimental data, and the turbulent burning speed is accurately predicted.

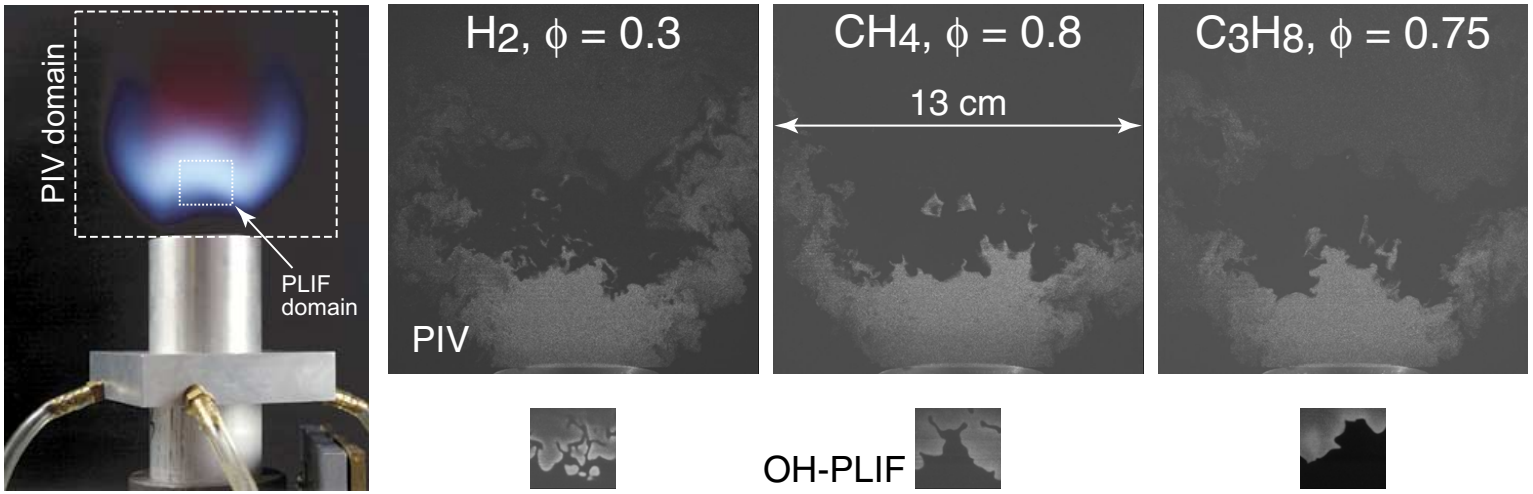
However the mean flame shape shows clear descrepancies

- The experimental flame is more squared off, consistent with a poorly characterized mean inflow
- We find flame shape sensitive to U_{coflow} as well

More detail is necessary to characterize the boundary data (mean fuel inflow and fluctuation spectra)

Example 2: Unattached Flames

Flame wrinkle structures from low-swirl experiment



- LSB used to gather data for turbulence/chemistry interactions
- (Apparent) local extinction, how to analyze experimental data?
- Can we use simulation to help understand these flames?

Classical Theory of Stretched Flames

Theory of (thin) premixed flames in open lab configurations:

$$s/s_L \sim 1 - Ma\,Ka$$

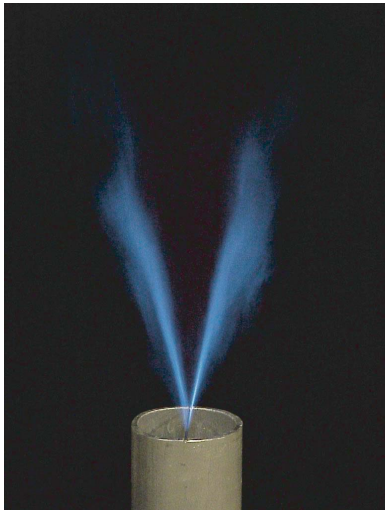
- s, the rate a flame overtakes premixed fuel
- s_L, the burning rate of the unstretched laminar flame
- Ka, normalized flame stretch (curvature and flow strain)
- Ma, the Markstein number $\rightarrow$ stability to flame wrinkling

Classically, Ma is determined by the transport properties of the deficient species (ie, CH_4 in lean CH_4/air flames)

But, CH_4/air flame experiments indicate sign change in Ma near $\phi = 0.75$

Precisely how does flame stretch modify the chemistry?

Laboratory Flame Stabilization



Rod-stabilized V-flame

4-jet Low-swirl burner (LSB)

Stagnation flame

Experimental configurations must overcome inherent instability

However, these devices complicate flame simulation

- How does stabilization effect the flame?
- Can we use a simple strategy to control the flame numerically?

Automatic Control of Premixed Turbulent Flames

Create idealized numerical configuration where we dynamically adjust mean inflow velocity to stabilize flame

Assumptions

- Flame location, x, defined using total mass of fuel in the domain
- There is an unknown turbulent flame speed $s(x)$ representing average speed of propagation that must be estimated
- Turbulent flame speed is not constant in time, it fluctuates around s

Stochastic ODE model

$$dx = (v_{in}(t) - s(x))dt + d\omega$$

Given an initial location of the flame $x(0) = \alpha$ and a target location β, find a strategy for adjusting $v_{in}(t)$ so that $x(t) \to \beta$ and estimate s

Want $v_{in}(t)$ to be smooth in time and positive

Control Strategy

Introduce time scale τ that defines target time to reach control.

Want τ sufficiently large that $\int_t^{t+\tau} d\omega \approx 0$

Given $v_{in}(t_0)$ and s_{est} solve

$$\beta = x(t_0) + \int_{t_0}^{t_0+\tau} v_{in}(t_0) + (t - t_0)\Delta v - s_{est}\, dt = \tau(v_{in}(t_0) - s_{est}) + \tau^2 \Delta v/2$$

for slope Δv to define linear profile for $v_{in}(t)$ that controls the solution to the desired target

Adjust Δv so that maximum change in v_{in} is limited and $v_{in} > 0$

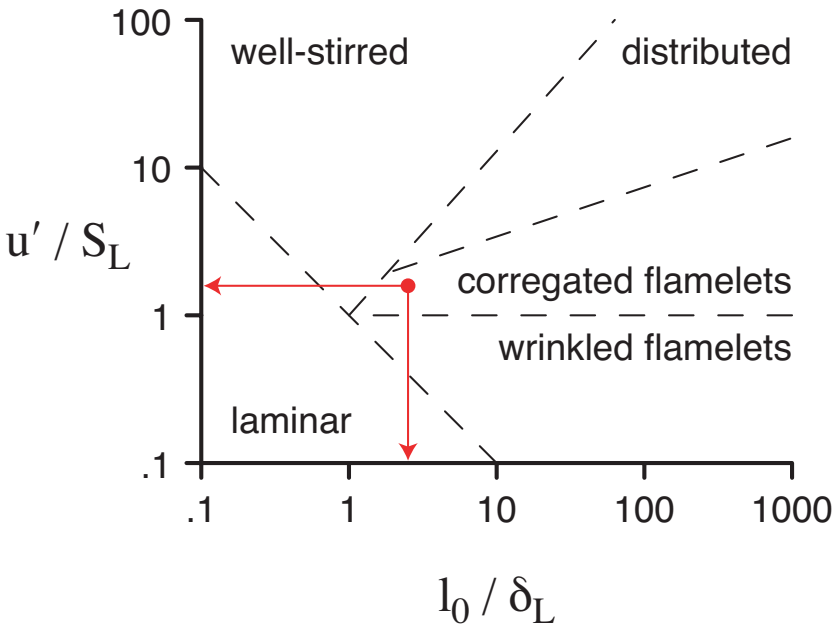
Use actual response of system to update s_{est}

$$s_{est} = (1 - \epsilon)s_{est} + \epsilon s_{obs}^{loc}$$

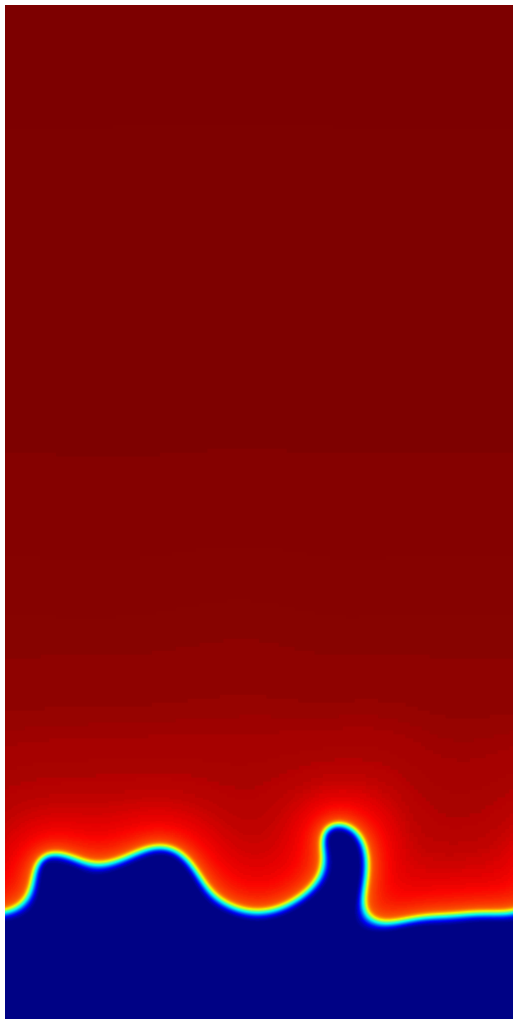
2D Application

Three “identical” flames

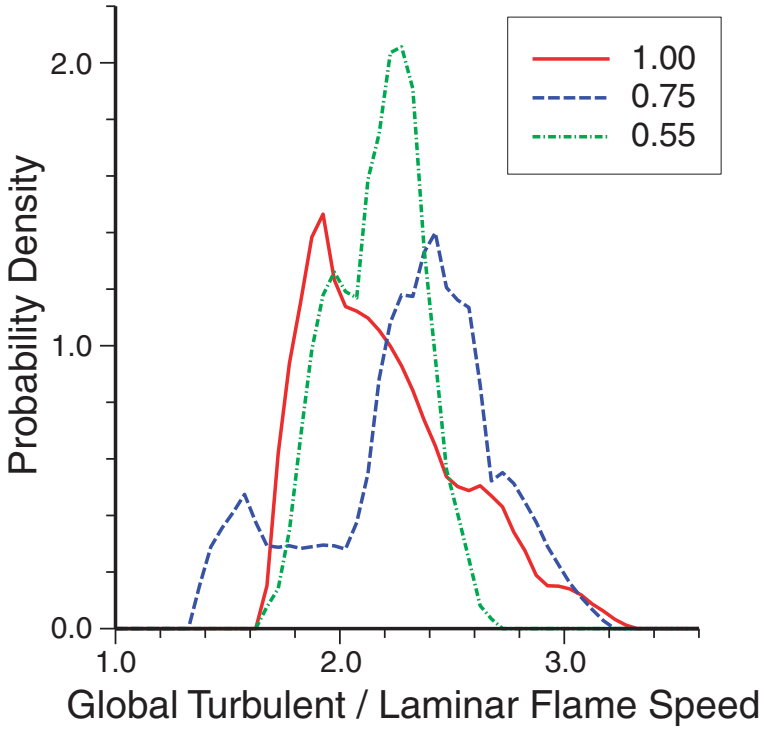
- ϕ = (0.55, 0.75, 1.00)
- $\ell_t \sim 2.6\delta_T$, $u' \sim 1.6 s_L$
- $L \sim 46\delta_T \sim 17\ell_t$
- $\Delta x = L/1024 \sim \delta_T/22$

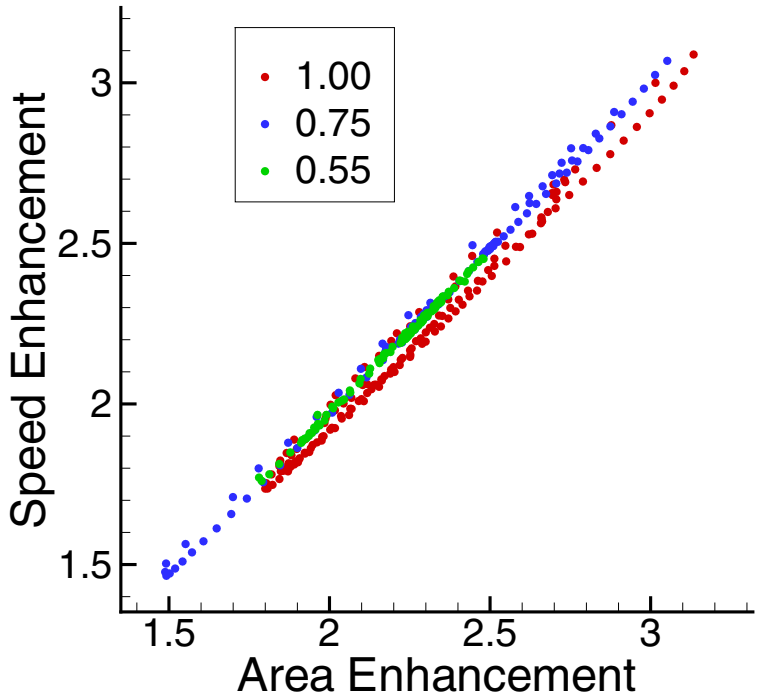


Example: $\phi = 1$



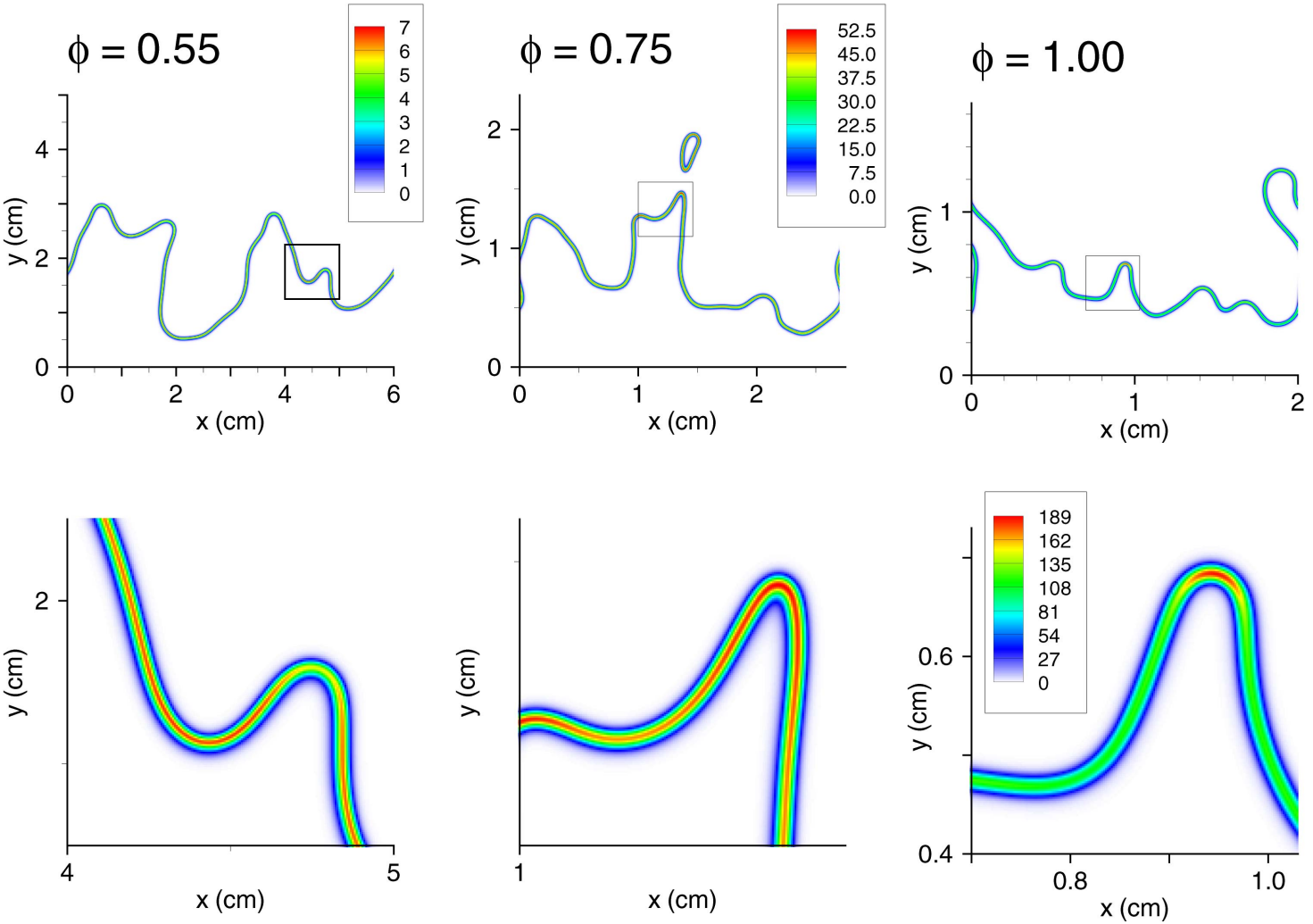
Turbulent Flame Speeds



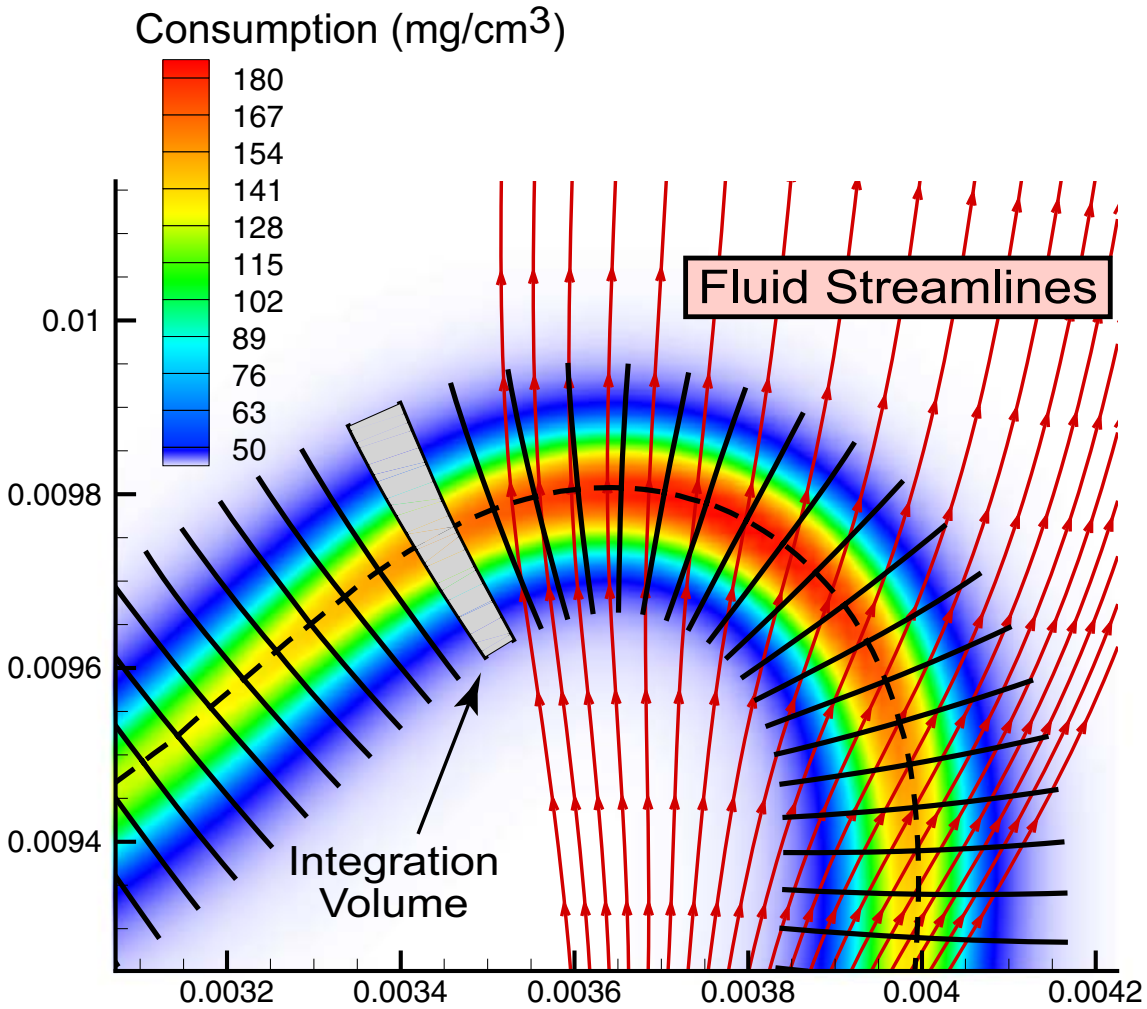


- Global burning speeds shows wide variability
- Correlates strongly with flame area in all cases

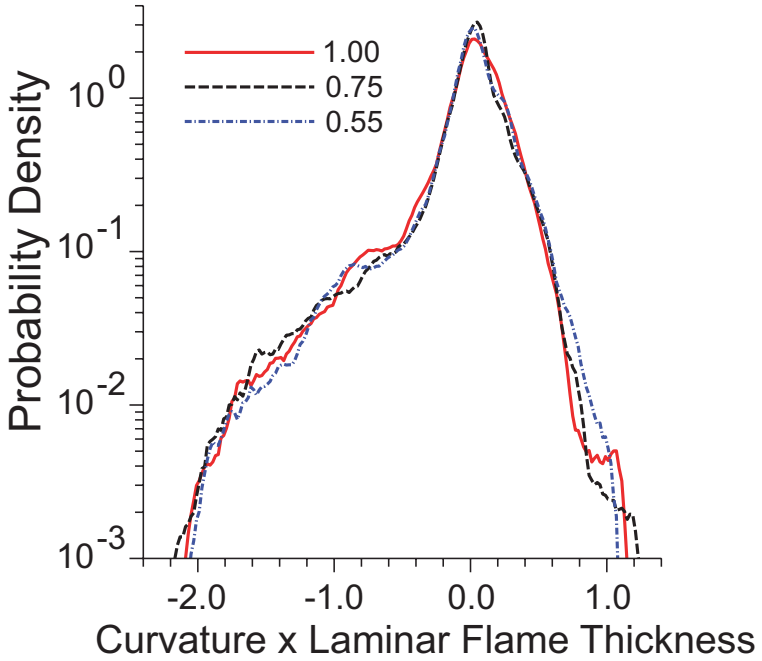
Consumption Rate Variability

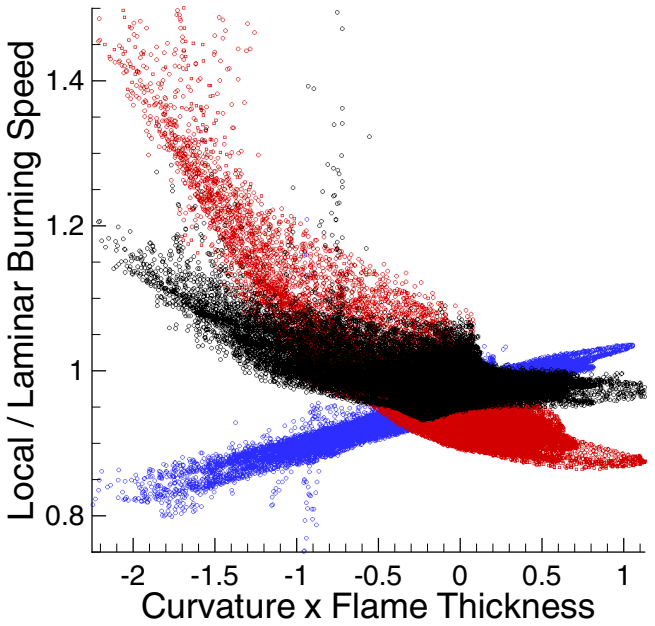


Local estimates of s_T



Local Flame Analysis





- Local flame curvature identical for all three flames (left-hand plot)
- *Ma* (slope of right-hand plot) agrees with experimental data
- Tangential strain rate (not shown here) not correlated with consumption

Can we quantify the effects of flow strain and flame curvature in terms of detailed chemical processes?

Lagrangian Pathline Analysis

Track moles per unit mass on pathlines in the flow along $\vec{v}(x,t)$

$$\rho \frac{DY_m}{Dt} = \nabla \cdot \rho D_m \nabla Y_m + \rho \dot{\omega}_m$$

Composition changes along path line due to

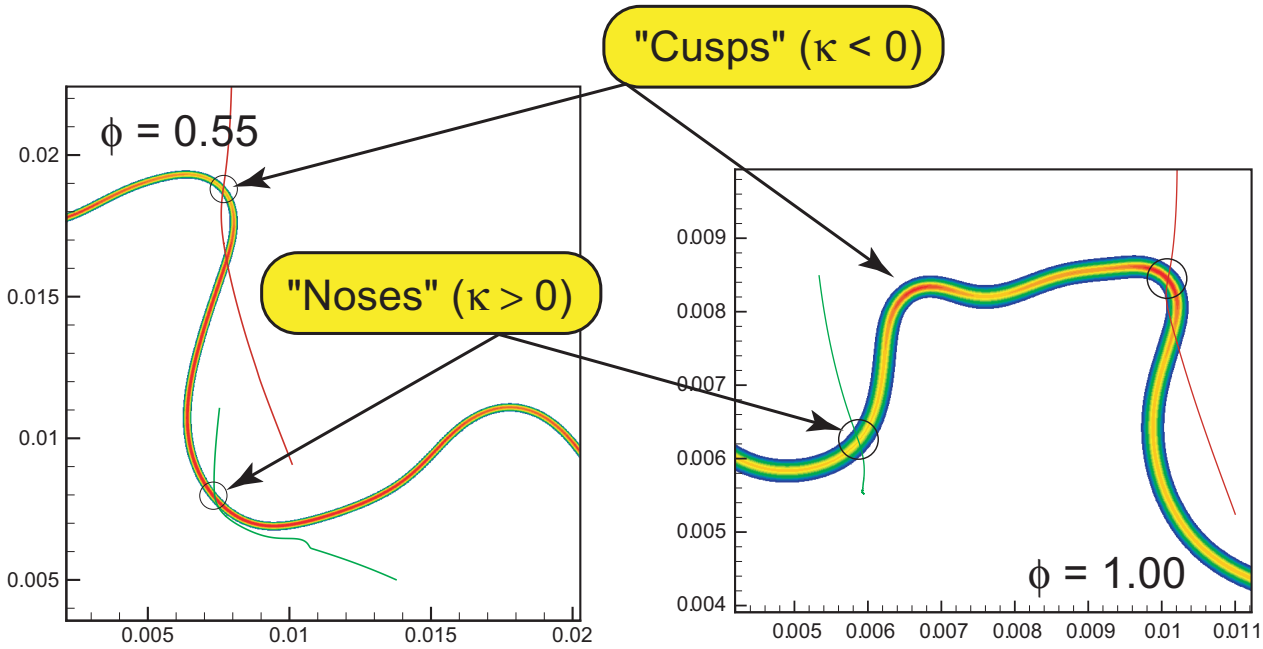
- Diffusive transport into pathline
- Chemical production

Given a time sequence of snapshots of the evolving simulation:

- Identify an "interesting" point in space-time, $\vec{x}_o$
- Construct a pathline through $\vec{x}_o$ by integrating $\vec{v}$ in time
- Sample the computed state along this pathline
- Given $\dot{\omega}(\vec{x})$ from the state along the pathline, solve inverse problem for diffusion source, $\mathcal{D}(\vec{x}) = (1/\rho)\nabla \rho D_m \nabla Y_m$

Methane Case

For GRIMech-3.0 (52 species, 325 reactions)



Dominant routes removing first H atom from CH_4:

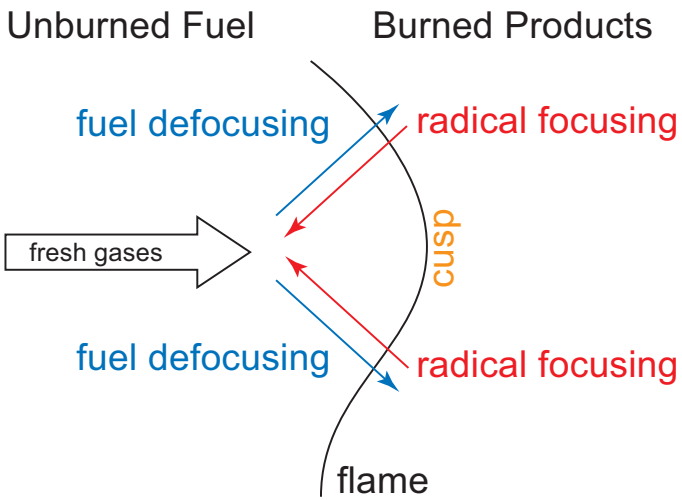
$$\textit{Rx}.\ 11: \quad O + CH_4 \rightleftharpoons OH + CH_3$$

$$\textit{Rx}.\ 52: \quad H + CH_3(+M) \rightleftharpoons CH_4(+M)$$

$$\textit{Rx}.\ 53: \quad H + CH_4 \rightleftharpoons CH_3 + H_2$$

$$\textit{Rx}.\ 98: \quad OH + CH_4 \rightleftharpoons CH_3 + H_2O$$

Competing Effects



For $\kappa < 0$ (cusp)

- Fuel defocused (drives down combustion rates)
- Radicals focused (drives up combustion rates)

The balance of these effects is determined by the extent to which highly mobile atoms play a role in the initial destruction of fuel atoms.

- For ϕ =1.00, H important, so radical focusing dominates
- For ϕ =0.55, H not so important, fuel loss dominates

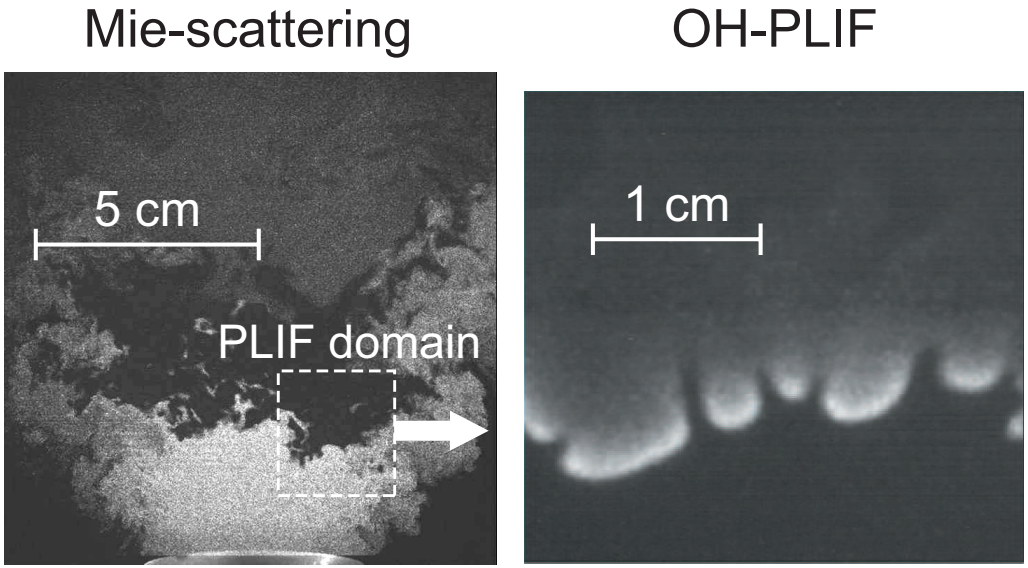
This is not related to the transport of CH_4, as suggested by classical theories(!)

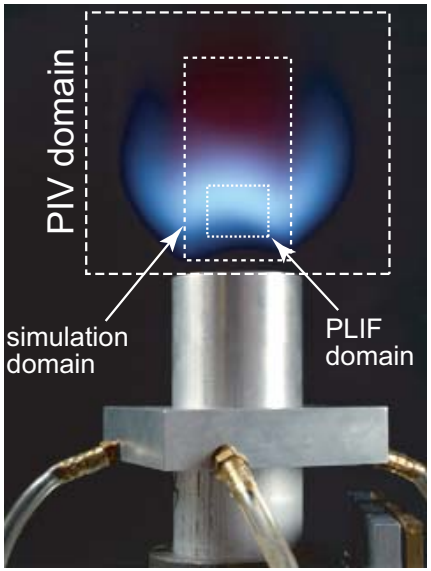
Hydrogen flame extinction

Mie-scattering shows 650K isotherm, OH-PLIF indicates combustion reactions

Lean H_2/air flames burn in cellular structures. $\longrightarrow$

(images courtesy R.K. Cheng)

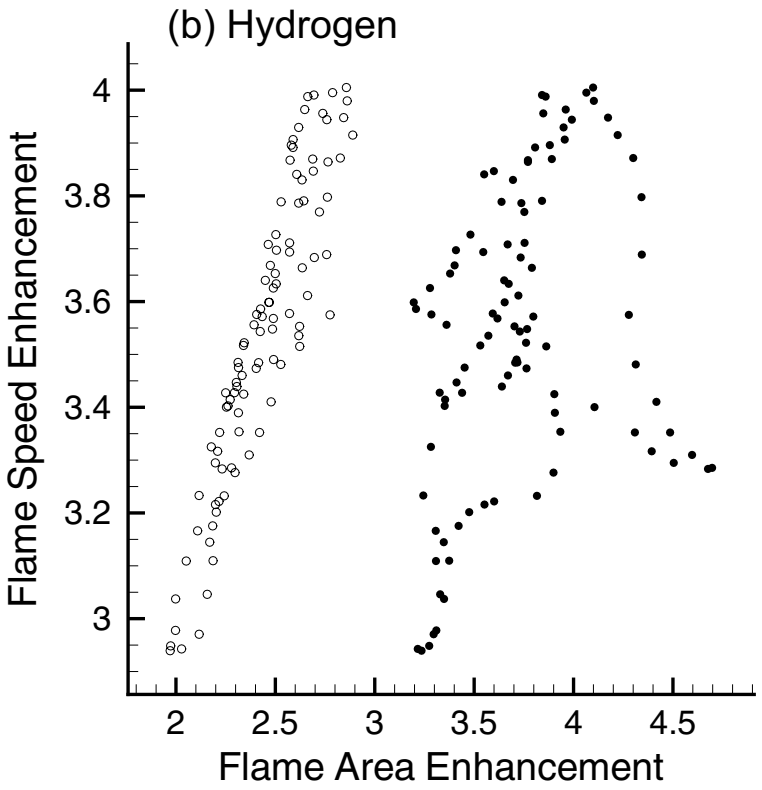


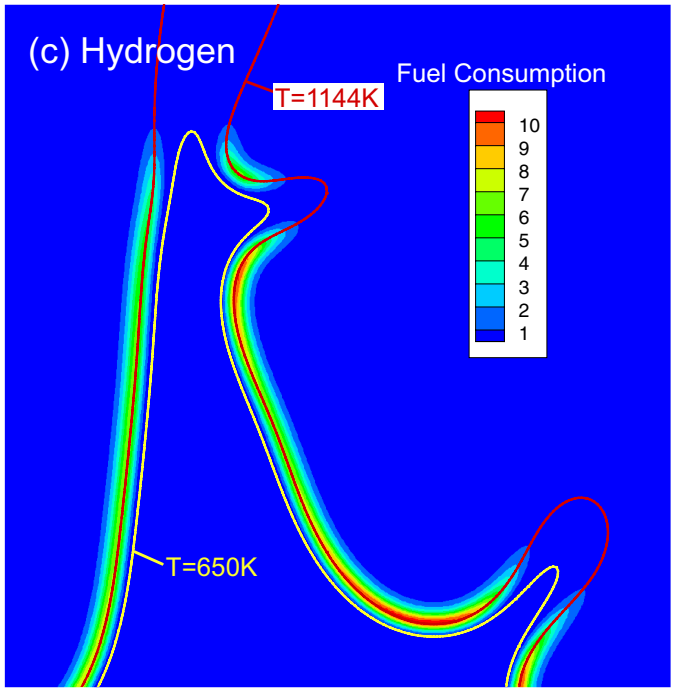


How do hydrogen flame extinguish? Does unburned fuel leak through?

The control strategy can be used to simulate the core region of the low swirl burner.

Flame Length vs. Turbulent Speed

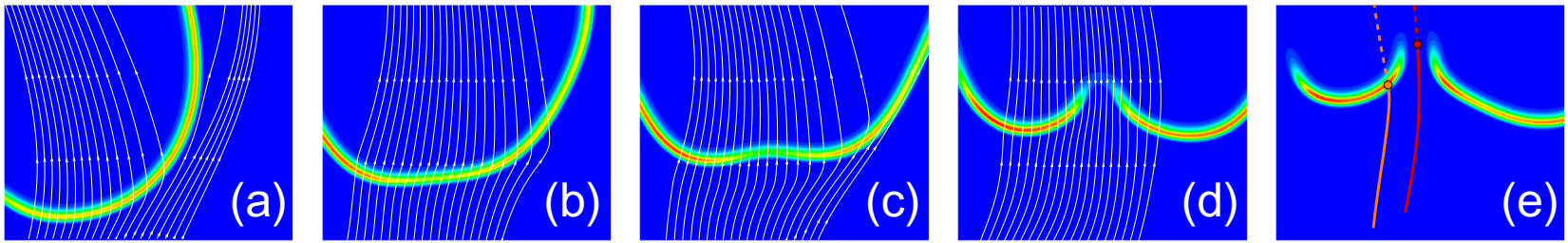




- Local and integrated burning enhanced dramatically over flat
- Which contour for area enhancement?
  650 K (PIV), 1144 K (peak consumption)
- Clearly this is not a “wrinkled laminar flamelet”

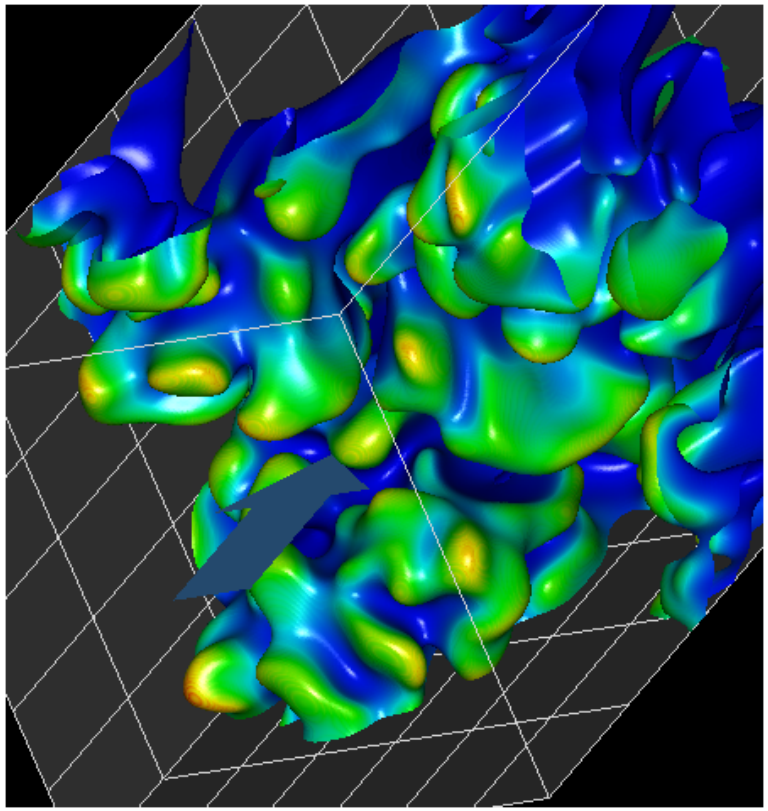
Localized Hydrogen Flame “Extinction”

Can we understand the development of the extinction pockets?

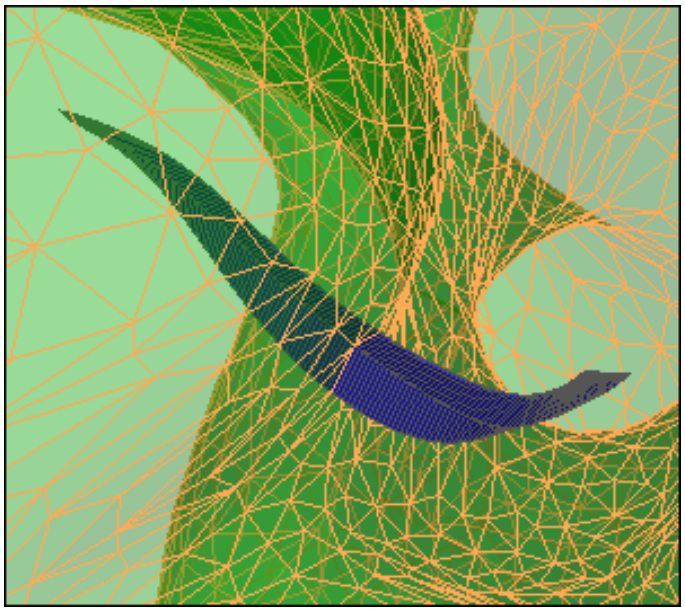


- Low-level localized strain event leads to onset of extinction.
- Features persist long after initial perturbation advects away.
- As a result, instantaneous correlations at (e) are deceiving
- Lagrangian analysis of differential diffusion suggests highly mobile fuel atoms diffuse “off-pathline”, no fuel leakage.
- Is there a correlation with turbulence parameters?
- How is this process affected in 3D?

Controlled 3D Hydrogen Flames



Cellular structures in a lean 3D H_2 flame

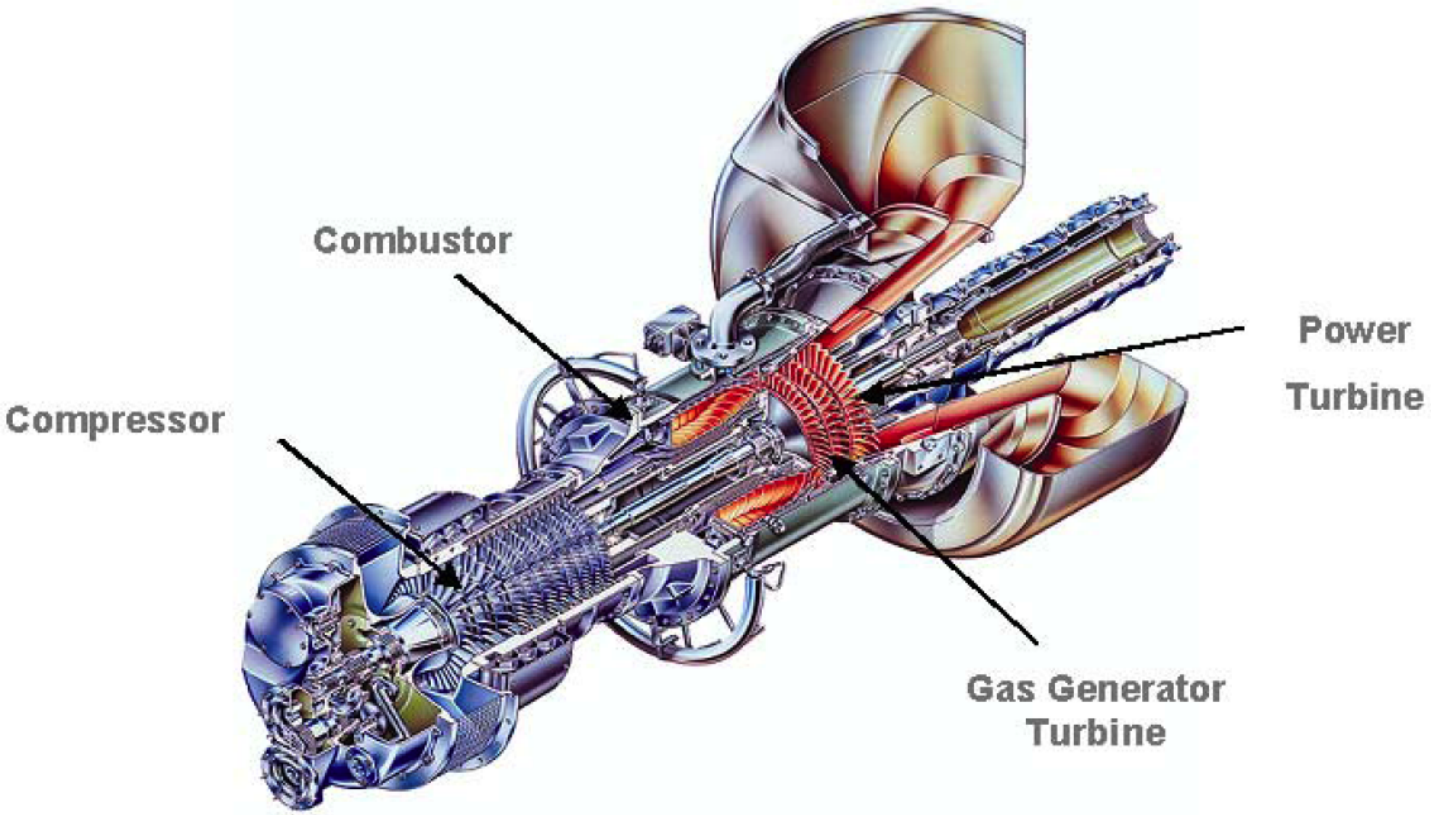


Flame surface analysis in 3D

- Local integrals through flame
- Bounding edges follow ∇T
- Typically $>$ 300K elements/step

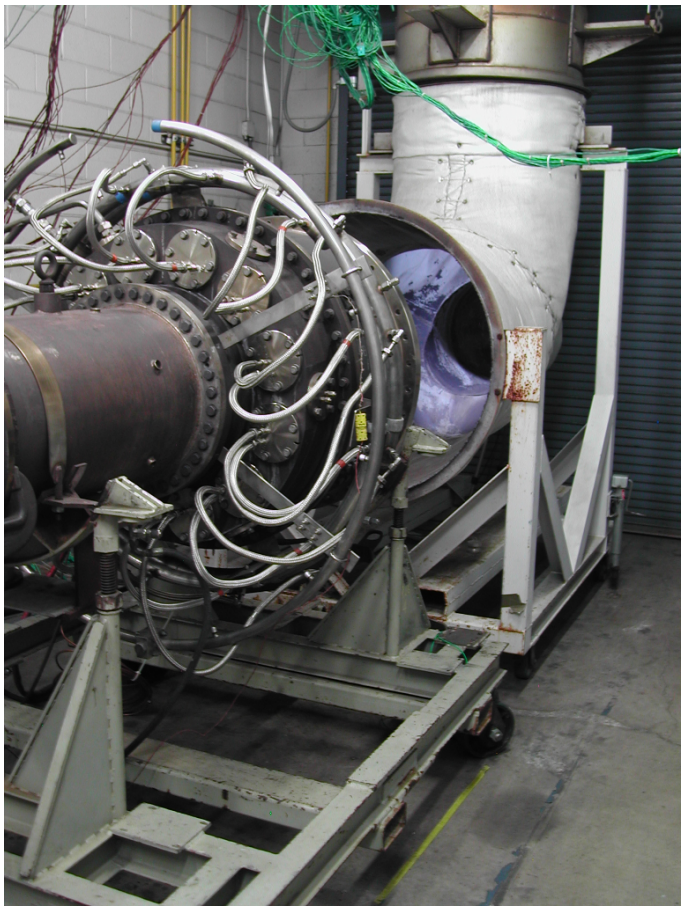
We are currently extending our 2D diagnostics to 3D.

Future directions



Turbine based on low-swirl burner technology

LSB-based turbine



Experimental rig to test array of 12 LSBs.

Future directions

Our future work will focus on more detailed simulations of fuel-flexible full-scale low-swirl burners

- Detailed transport/chemistry - Larger runs, harder analysis
  - Pollutant generation
  - Higher-order transport (binary diffusion, Dufour/Soret transport)
- Complete configurations - validation, analysis, geometry
  - Realistic inflowing turbulence
  - High-pressure, temperature
  - Closed combustor
- Geometry - visualization/analysis, algorithms
  - Multiple burners
  - Vessel geometry
  - Acoustics

Practical Observations

1. Data Management: Current research generates $\mathcal{O}$(5 TB) raw data per study, requires frequent repeated access of subsets. This will increase significantly in the next couple of years. Our current processing stream is demand-driven, but entire dataset must be resident on disk.

2. Performance Analysis: I/O, parallelism, node performance and debugging are extremely difficult for $\mathcal{O}(10^2 - 10^3)$ processors. We can only imagine how much harder this will be for $\mathcal{O}(10^4 - 10^5)$ processors!

3. Visualization/Analysis: We have found very few useful remote data subsetting approaches based on high-performance visualization. We must compute on subsets, not just display them. To date, we write our own extractions and view them locally with Tecplot/IDL/etc. This solution is not scalable, or extensible.